



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 06:52 PM BST

PDB ID : 6YUB  
Title : Crystal structure of Uba4 from Chaetomium thermophilum  
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Deposited on : 2020-04-26  
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

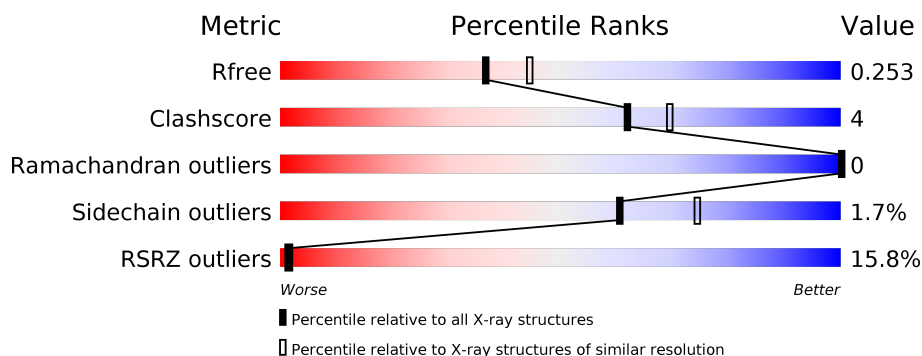
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	442	<div> <div>12%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
2	B	303	<div> <div>3%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
3	C	127	<div> <div>55%</div> <div>79%</div> <div>9%</div> <div>12%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12369 atoms, of which 6048 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adenylyltransferase and sulfurtransferase uba4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	423	Total	C	H	N	O	S	1	6	0
			6264	1982	3122	548	589	23			

- Molecule 2 is a protein called Adenylyltransferase and sulfurtransferase uba4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	289	Total	C	H	N	O	S	0	6	0
			4328	1362	2183	371	394	18			

- Molecule 3 is a protein called Adenylyltransferase and sulfurtransferase uba4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	112	Total	C	H	N	O	S	0	0	0
			1553	510	743	146	151	3			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	93	Total	O	0	0
			93	93		
5	B	116	Total	O	0	0
			116	116		

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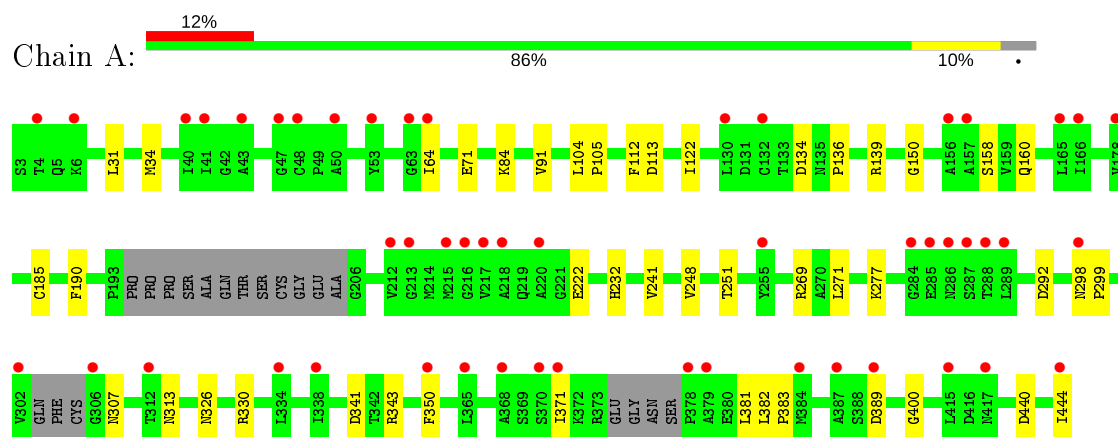
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	13	Total	O	0	0
			13	13		

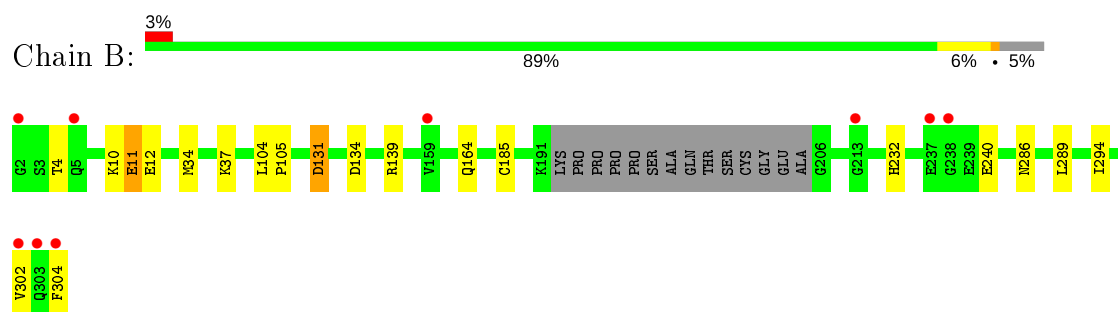
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

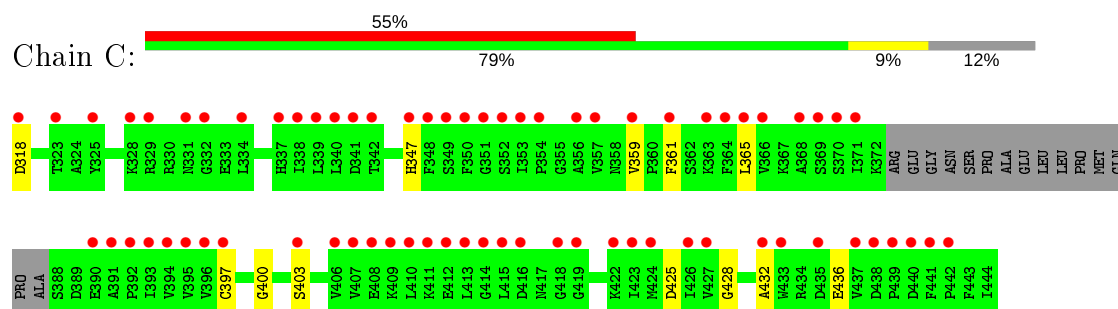
- Molecule 1: Adenylyltransferase and sulfurtransferase uba4



- Molecule 2: Adenylyltransferase and sulfurtransferase uba4



- Molecule 3: Adenylyltransferase and sulfurtransferase uba4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.75Å 74.17Å 103.66Å 90.00° 106.36° 90.00°	Depositor
Resolution (Å)	47.63 – 2.19 47.63 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.63-2.19) 99.5 (47.63-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.208 , 0.253 0.208 , 0.253	Depositor DCC
$R_{free}$ test set	2405 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.31	0/3204	0.46	0/4350
2	B	0.35	1/2193 (0.0%)	0.48	1/2977 (0.0%)
3	C	0.26	0/824	0.41	0/1117
All	All	0.32	1/6221 (0.0%)	0.46	1/8444 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	11	GLU	CG-CD	5.81	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	11	GLU	OE1-CD-OE2	-6.30	115.73	123.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3142	3122	3108	30	1
2	B	2145	2183	2166	11	1
3	C	810	743	740	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	93	0	0	9	2
5	B	116	0	0	5	1
5	C	13	0	0	3	0
All	All	6321	6048	6014	53	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:O	5:B:501:HOH:O	1.84	0.94
2:B:164:GLN:NE2	5:B:505:HOH:O	2.05	0.90
3:C:347:HIS:ND1	5:C:501:HOH:O	2.06	0.88
2:B:4:THR:O	5:B:502:HOH:O	1.94	0.86
1:A:400:GLY:O	5:A:601:HOH:O	1.96	0.83
1:A:160:GLN:O	5:A:602:HOH:O	2.03	0.75
2:B:240:GLU:O	5:B:504:HOH:O	2.04	0.75
1:A:134:ASP:OD2	5:A:603:HOH:O	2.04	0.75
3:C:397:CYS:SG	5:C:505:HOH:O	2.45	0.74
3:C:361:PHE:O	3:C:365:LEU:HD12	1.95	0.66
1:A:371:ILE:HG22	1:A:371:ILE:O	1.96	0.65
1:A:222:GLU:OE2	5:A:604:HOH:O	2.14	0.64
1:A:113:ASP:OD2	5:A:605:HOH:O	2.15	0.63
3:C:361:PHE:CZ	3:C:365:LEU:HD11	2.35	0.61
1:A:381:LEU:C	1:A:383:PRO:HD2	2.23	0.58
2:B:289:LEU:HD11	2:B:294:ILE:HD11	1.84	0.58
1:A:382:LEU:N	1:A:383:PRO:HD2	2.19	0.57
1:A:31:LEU:HD23	1:A:34:MET:CE	2.34	0.57
3:C:359:VAL:HG23	3:C:359:VAL:O	2.05	0.57
1:A:136:PRO:HG3	1:A:307:ASN:HA	1.87	0.56
2:B:37:LYS:NZ	5:B:503:HOH:O	2.00	0.56
1:A:298:ASN:HB3	1:A:299:PRO:HD3	1.88	0.55
1:A:350:PHE:CG	1:A:444:ILE:HD11	2.42	0.54
1:A:241:VAL:HG21	1:A:248:VAL:HG23	1.90	0.53
1:A:112:PHE:HE2	1:A:122:ILE:HD11	1.74	0.52
1:A:71:GLU:OE1	5:A:606:HOH:O	2.19	0.52
1:A:382:LEU:N	1:A:383:PRO:CD	2.72	0.52
2:B:12:GLU:OE2	2:B:34:MET:HE3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:318:ASP:N	5:C:504:HOH:O	2.46	0.49
1:A:277:LYS:HE3	1:A:313:ASN:HB3	1.95	0.48
2:B:12:GLU:OE2	2:B:34:MET:CE	2.61	0.48
3:C:403:SER:HB3	3:C:425:ASP:HB2	1.96	0.48
1:A:150:GLY:HA2	5:A:655:HOH:O	2.14	0.47
3:C:428:GLY:HA3	3:C:432:ALA:HB2	1.96	0.47
1:A:84:LYS:HG3	5:A:656:HOH:O	2.13	0.47
3:C:397:CYS:SG	3:C:400:GLY:N	2.89	0.46
2:B:104:LEU:N	2:B:105:PRO:CD	2.79	0.45
1:A:326:ASN:O	1:A:330:ARG:HG2	2.17	0.44
3:C:361:PHE:CE1	3:C:365:LEU:HD11	2.52	0.44
1:A:350:PHE:CD1	1:A:444:ILE:HD11	2.52	0.44
1:A:104:LEU:N	1:A:105:PRO:CD	2.81	0.44
3:C:432:ALA:HB1	3:C:436:GLU:OE1	2.18	0.43
2:B:302:VAL:HG13	2:B:304:PHE:CE1	2.54	0.43
2:B:131:ASP:OD2	2:B:139:ARG:HG2	2.19	0.42
1:A:190:PHE:HB3	5:A:631:HOH:O	2.20	0.41
1:A:64:ILE:HB	1:A:91:VAL:HG23	2.02	0.41
1:A:341:ASP:OD1	1:A:343:ARG:HD3	2.21	0.41
3:C:361:PHE:CE2	3:C:365:LEU:HD11	2.56	0.41
1:A:139:ARG:NH2	1:A:307:ASN:O	2.54	0.41
1:A:158:SER:O	1:A:307:ASN:ND2	2.53	0.41
1:A:269[A]:ARG:HD3	1:A:271:LEU:HD21	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:682:HOH:O	5:A:693:HOH:O[1_455]	1.80	0.40
1:A:269[B]:ARG:NH2	2:B:286:ASN:OD1[2_646]	2.07	0.13
5:A:691:HOH:O	5:B:591:HOH:O[2_546]	2.08	0.12

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/442 (94%)	396 (95%)	21 (5%)	0	100	100
2	B	287/303 (95%)	277 (96%)	10 (4%)	0	100	100
3	C	108/127 (85%)	104 (96%)	4 (4%)	0	100	100
All	All	812/872 (93%)	777 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/369 (90%)	329 (98%)	5 (2%)	65	78
2	B	232/250 (93%)	226 (97%)	6 (3%)	46	58
3	C	76/108 (70%)	76 (100%)	0	100	100
All	All	642/727 (88%)	631 (98%)	11 (2%)	60	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185[4]	CYS
1	A	232	HIS
1	A	292	ASP
1	A	389	ASP
1	A	440	ASP
2	B	10	LYS
2	B	11	GLU
2	B	131	ASP
2	B	134	ASP
2	B	185[3]	CYS
2	B	232	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	164	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	423/442 (95%)	0.96	51 (12%) 4 3	28, 49, 90, 144	2 (0%)
2	B	289/303 (95%)	0.55	9 (3%) 49 47	27, 39, 66, 120	0
3	C	112/127 (88%)	3.05	70 (62%) 0 0	59, 84, 116, 150	0
All	All	824/872 (94%)	1.10	130 (15%) 2 1	27, 46, 102, 150	2 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	371	ILE	10.9
3	C	350	PHE	7.1
3	C	369	SER	7.1
3	C	334	LEU	7.0
3	C	414	GLY	7.0
3	C	441	PHE	6.9
3	C	423	ILE	6.7
2	B	304	PHE	6.5
3	C	370	SER	6.4
3	C	442	PRO	6.2
3	C	413	LEU	5.8
3	C	340	LEU	5.8
2	B	303	GLN	5.6
3	C	395	VAL	5.6
3	C	407	VAL	5.5
3	C	366	VAL	5.4
3	C	364	PHE	5.4
2	B	302	VAL	5.3
3	C	338	ILE	5.3
3	C	353	ILE	5.3
3	C	368	ALA	5.1
3	C	439	PRO	5.0
3	C	396	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
3	C	418	GLY	4.8
1	A	415	LEU	4.7
3	C	410	LEU	4.7
3	C	422	LYS	4.6
3	C	357	VAL	4.6
3	C	352	SER	4.5
3	C	411	LYS	4.5
3	C	390	GLU	4.3
3	C	415	LEU	4.3
3	C	359	VAL	4.2
3	C	394	VAL	4.1
3	C	337	HIS	4.1
1	A	387	ALA	4.1
3	C	325	TYR	4.1
1	A	178	VAL	4.0
1	A	378	PRO	4.0
3	C	342	THR	4.0
1	A	371	ILE	3.8
1	A	50	ALA	3.8
3	C	409	LYS	3.7
3	C	349	SER	3.7
3	C	332	GLY	3.7
1	A	298	ASN	3.7
1	A	289	LEU	3.6
3	C	339	LEU	3.6
3	C	416	ASP	3.6
1	A	368	ALA	3.5
1	A	444	ILE	3.5
1	A	48	CYS	3.5
3	C	412	GLU	3.5
1	A	287	SER	3.5
1	A	156	ALA	3.4
3	C	365	LEU	3.4
1	A	417	ASN	3.4
1	A	370	SER	3.3
3	C	331	ASN	3.3
3	C	393	ILE	3.3
1	A	306	GLY	3.2
3	C	348	PHE	3.2
3	C	351	GLY	3.2
3	C	427	VAL	3.1
3	C	391	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	361	PHE	3.1
3	C	419	GLY	3.0
3	C	438	ASP	3.0
3	C	406	VAL	3.0
3	C	403	SER	3.0
1	A	43	ALA	3.0
3	C	440	ASP	2.9
1	A	212	VAL	2.9
2	B	159	VAL	2.9
1	A	288	THR	2.9
3	C	318	ASP	2.9
1	A	218	ALA	2.8
1	A	379	ALA	2.8
1	A	389	ASP	2.7
3	C	408	GLU	2.7
1	A	334	LEU	2.6
1	A	47	GLY	2.6
1	A	384	MET	2.6
1	A	220	ALA	2.6
1	A	338	ILE	2.6
1	A	130	LEU	2.6
3	C	392	PRO	2.6
3	C	323	THR	2.5
3	C	435	ASP	2.5
1	A	217	VAL	2.5
3	C	356	ALA	2.5
1	A	4	THR	2.5
2	B	238	GLY	2.5
3	C	354	PRO	2.5
1	A	216	GLY	2.5
1	A	284	GLY	2.5
3	C	424	MET	2.4
3	C	347	HIS	2.4
1	A	312	THR	2.4
1	A	286	ASN	2.4
2	B	237	GLU	2.4
3	C	432	ALA	2.4
1	A	213	GLY	2.4
3	C	433	TRP	2.4
1	A	132	CYS	2.4
2	B	213	GLY	2.3
3	C	437	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	40	ILE	2.3
1	A	165	LEU	2.3
2	B	2	GLY	2.3
1	A	64	ILE	2.2
3	C	329	ARG	2.2
1	A	41	ILE	2.2
3	C	397	CYS	2.1
1	A	157	ALA	2.1
3	C	363	LYS	2.1
1	A	6	LYS	2.1
1	A	302	VAL	2.1
3	C	341	ASP	2.1
2	B	5	GLN	2.1
3	C	426	ILE	2.1
1	A	255	TYR	2.1
1	A	365	LEU	2.0
3	C	328	LYS	2.0
1	A	350	PHE	2.0
1	A	215	MET	2.0
1	A	53	TYR	2.0
1	A	285	GLU	2.0
1	A	166	ILE	2.0
1	A	63	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

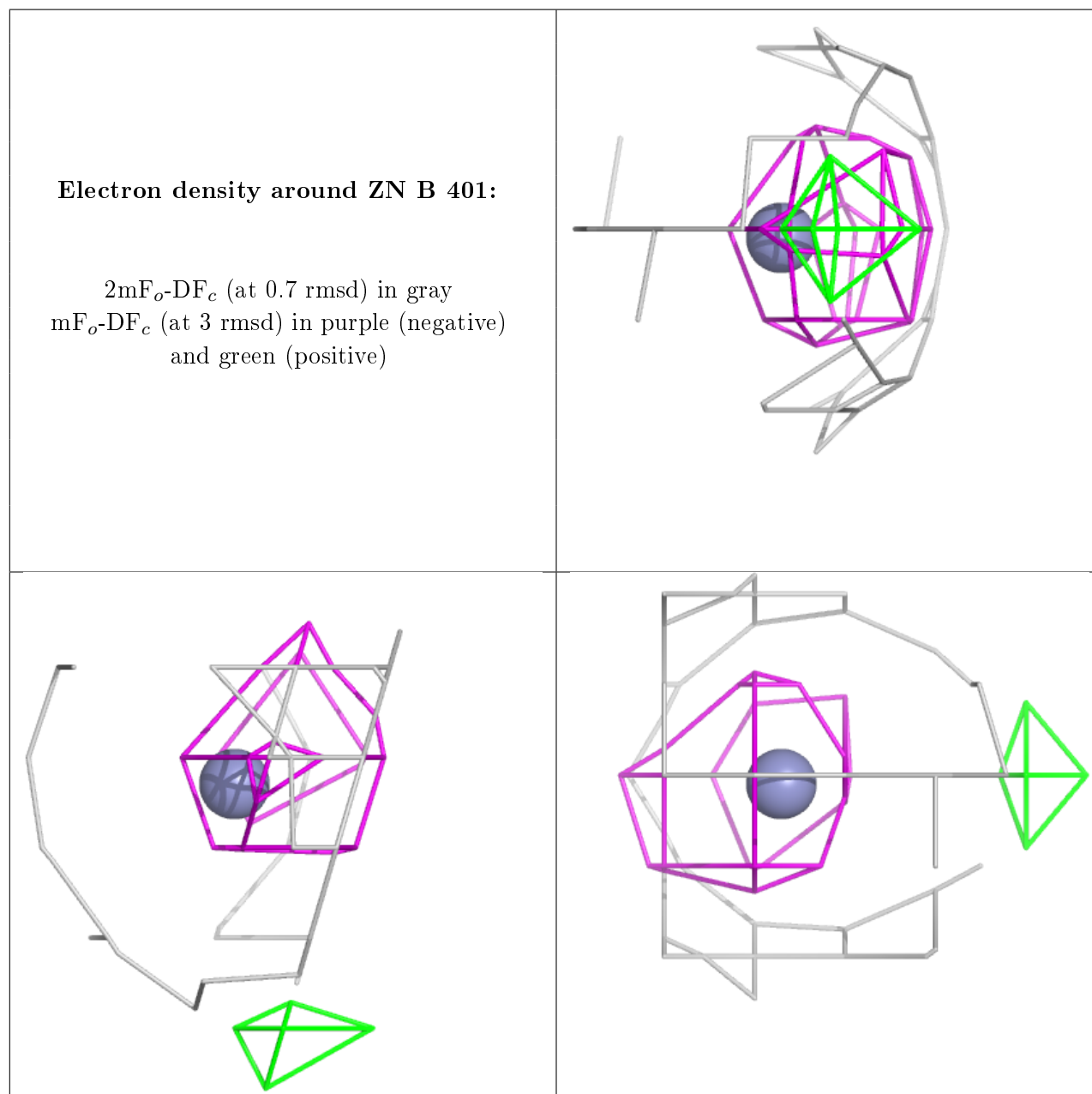
*Continued on next page...*

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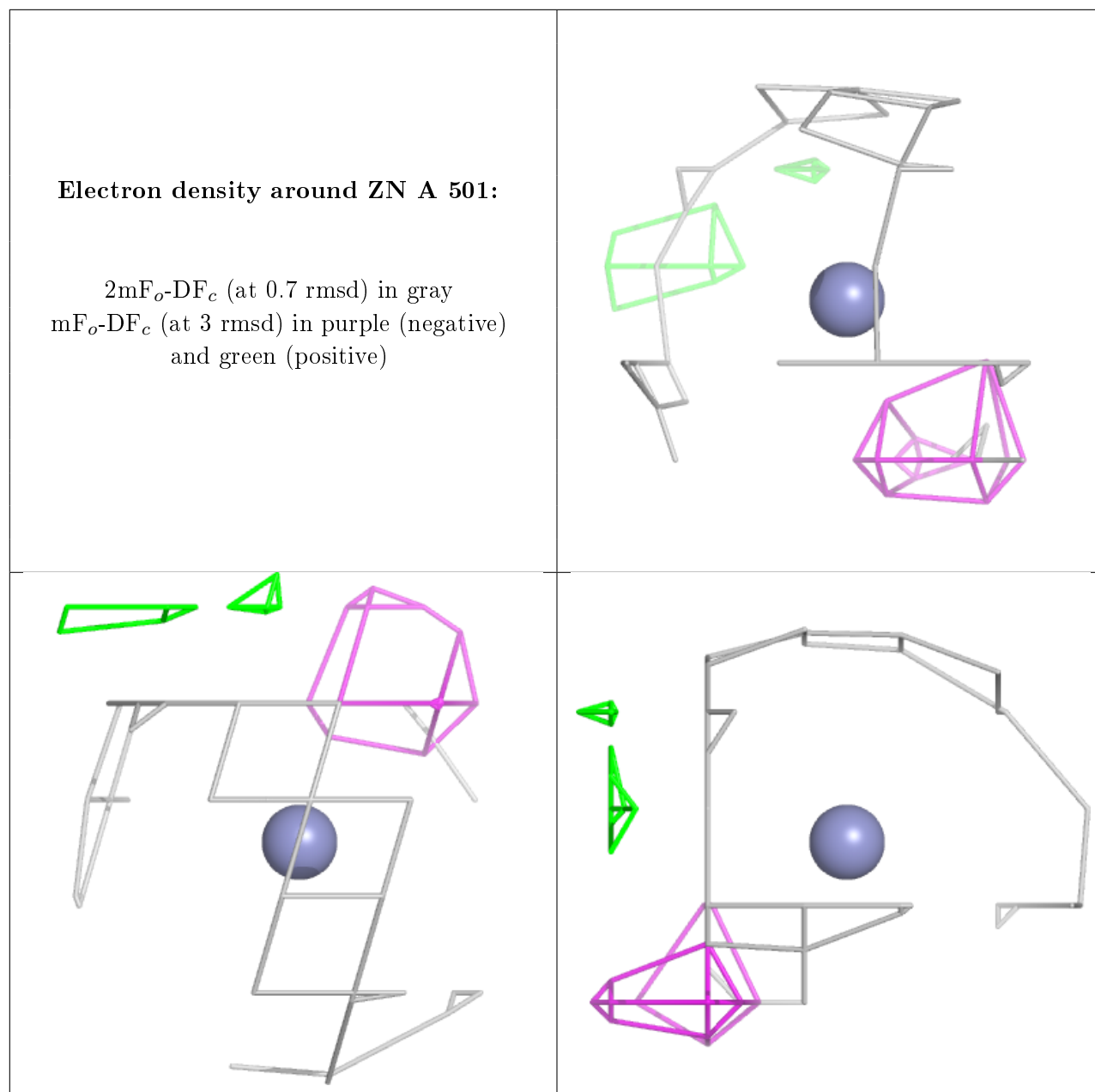
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	B	401	1/1	0.99	0.08	38,38,38,38	0
4	ZN	A	501	1/1	0.99	0.10	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







## 6.5 Other polymers ⓘ

There are no such residues in this entry.